Title: Raman optical activity and conformational flexibility of peptides in solution

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Abstract: Molecular flexibility can significantly modify Raman and ROA spectral intensities, band positions and the ROA signs. Taking into account dynamic aspects of behavior of studied molecules in solution via conformational averaging therefore seems to be crucial for spectral interpretation. The first of studied models, histidine, plays an important role in metallo-enzymatic reactions and peptide folding, due to its imidazole ring. ROA spectra of His at different pH, His complexed with Cu^{2+} and dipeptides His-Gly and Gly-His were recorded on the spectrometer built at the Institute of Physics of the Charles University as a first step of the subsequent study. The second studied system, a cyclic hexapeptide c-(Phe-D-Pro-Gly-Arg-Gly-Asp), serves as a convenient model for β-hairpin and anti-parallel β-sheet. It was previously studied by means of VCD and IR. From molecular dynamics simulations 10 peptide geometries were selected for spectral modeling. The Raman and ROA spectra were calculated *ab initio*. For a model fragment Phe-D-Pro, which dominates in the Raman spectrum, Boltzmann averaging over 36 conformations has been done.

Keywords: Raman optical activity, conformational flexibility, β-turn, cyclic peptide, histidin